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# (*E*)-1-[(2-Chlorophenyl)methyleneamino]guanidinium chloride

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**Key indicators**

Single-crystal X-ray study
*T* = 90 K
Mean *σ*(C–C) = 0.004 Å
*R* factor = 0.053
*wR* factor = 0.141
Data-to-parameter ratio = 18.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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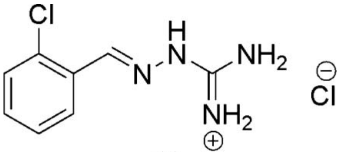
The title compound, $C_8H_{10}ClN_4^+\cdot Cl^-$, was prepared by the condensation reaction of 2-chlorobenzaldehyde with aminoguanidine hydrochloride. The guanidinium group is twisted by 21.88 (17)° from the 2-chlorophenyl ring and the C═N group has *E* geometry. The chloride ions are involved in intermolecular hydrogen bonds with the H atoms of the aminoguanidinium ion.

## Comment

Guanylhydrazones are derived from arylaldehydes and aminoguanidine, and exhibit a wide range of biological activities. An important representative of this class of compounds is the centrally acting antihypertensive agent guanabenz (2,6-dichlorobenzylideneaminoguanidine), used for the treatment of high blood pressure (Baum *et al.*, 1969). In view of their biological activities, we have synthesized a series of guanylhydrazones. The title compound, (I), was synthesized by the condensation reaction of 2-chlorobenzaldehyde with aminoguanidine hydrochloride under reflux in methanol, to afford a single geometrical isomer. The present X-ray crystallographic determination was carried out in order to confirm the C7═N1 double-bond geometry, and to obtain more detailed information on the conformation of the cation.



(I)

The molecular structure of (I) is shown in Fig. 1, and selected geometric parameters are presented in Table 1. The C7═N1 double bond connecting the guanidinium moiety with the 2-chlorophenyl ring system has *E* geometry. The plane of the guanidinium moiety is twisted from the plane of the 2-cholorophenyl ring by 21.88 (17)°, although there still exists partial conjugation between these moieties, as indicated by the C6—C7 bond length [1.472 (4) Å], which is comparable with the standard length for a $C_{ar}—Csp^2$ single bond [1.470 (15) Å; Allen *et al.*, 1987]. In the crystal structure, chloride ions interact *via* hydrogen bonding with the NH groups of the guanidinium ions. The geometric hydrogen-bonding parameters are listed in Table 2.

## Experimental

A mixture of 2-chlorobenzaldehyde (2.80 mg, 2.0 mmol) and aminoguanidine hydrochloride (144 mg, 1.3 mmol) was taken up in

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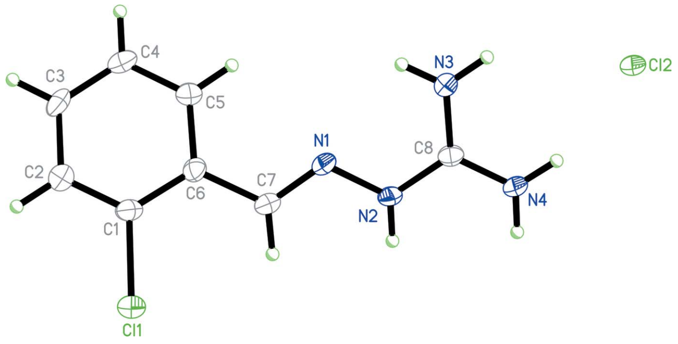

**Figure 1**
The molecular structure of (I) with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radius.

methanol (15 ml) and the mixture was refluxed for 8 h. After evaporation of solvent, the residue was stirred in chloroform and filtered to remove unreacted 2-chlorobenzaldehyde from the filtrate. The solid product was dried and recrystallized with 2-propanol.

### *Crystal data*

$C_8H_{10}ClN_4^+\cdot Cl^-$
$M_r = 233.10$
Monoclinic, $P2_1/c$
$a = 16.5020$ (14) Å
$b = 7.2234$ (5) Å
$c = 8.5816$ (6) Å
$\beta = 100.768$ (3)°
$V = 1004.92$ (13) Å$^3$
$Z = 4$
$D_x = 1.541$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 0.61$ mm$^{-1}$
$T = 90.0$ (2) K
Plate, colorless
0.30 × 0.20 × 0.05 mm

### *Data collection*

Nonius KappaCCD diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
$T_{\min} = 0.838$, $T_{\max} = 0.970$
7124 measured reflections
2296 independent reflections
1481 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.087$
$\theta_{\max} = 27.5°$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.141$
$S = 1.03$
2296 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 0.5156P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.57$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.45$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C1—Cl1 | 1.745 (3) | C8—N4 | 1.323 (4) |
| C6—C7 | 1.472 (4) | C8—N2 | 1.347 (4) |
| C8—N3 | 1.319 (4) | N1—N2 | 1.373 (3) |
| N1—C7—C6 | 118.8 (3) | C7—N1—N2 | 117.0 (2) |
| N3—C8—N4 | 121.1 (3) | C8—N2—N1 | 117.4 (2) |
| Cl1—C1—C6—C5 | 178.5 (2) | C5—C6—C7—N1 | 19.0 (5) |
| Cl1—C1—C6—C7 | 4.0 (5) | N4—C8—N2—N1 | 174.6 (3) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···Cl2$^{\rm i}$ | 0.88 | 2.50 | 3.230 (3) | 140 |
| N3—H3*A*···Cl2$^{\rm ii}$ | 0.88 | 2.61 | 3.221 (3) | 127 |
| N3—H3*B*···Cl2$^{\rm iii}$ | 0.88 | 2.61 | 3.297 (3) | 135 |
| N4—H4*A*···Cl2 | 0.88 | 2.40 | 3.197 (3) | 152 |
| N4—H4*B*···Cl2$^{\rm i}$ | 0.88 | 2.61 | 3.305 (3) | 137 |

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x, -y, -z+2$; (iii) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$.

H atoms were positioned geometrically and treated as riding, with C—H = 0.95 Å, N—H = 0.88 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(C,N).

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1995); software used to prepare material for publication: *SHELXL97*, and local procedures.

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